CROSS TOKAI Experimental Report J-PARC	承認日 Date of Approval: 2016/1/18 承認者 Approver: Ryoichi Kajimoto 提出日 Date of Report: 2016/1/18
実験課題番号 Project No. 2014P0901 実験課題名 Title of experiment Project research on protonic, superionic and amorphous functional materials using 4SEASONS 実験責任者名 Name of principal investigator Mitsutaka Nakamura 所属 Affiliation Japan Atomic Energy Agency	装置責任者 Name of Instrument scientist Ryoichi Kajimoto 装置名 Name of Instrument/（BL No.） 4SEASONS (BL01) 利用期間 Dates of experiments 2014/11/19 21：00 – 2014/11/23 11:00 2014/12/12 11：00 – 2014/12/15 11:00

1．研究成果概要（試料の名称、組成、物理的・化学的性状を明記するとともに、実験方法、利用の結果得られた主なデータ、考察、結論、図表等を記述してください。

Outline of experimental results (experimental method and results should be reported including sample information such as composition, physical and/or chemical characteristics.

Sample Information

2014A: $Ba_8Ga_{16}Sn_{30}$ single crystals

2014B: ScF_3 powder

Experimental Condition

2014A: Fermi 200Hz, E_i=12.0, 20.6, 41.8, 130.0 meV (multi-E_i); RT; rotating crystal measurement

2014B: Fermi 250Hz, E_i=15.8, 25.5, 42.9, 121.1 meV (multi-E_i); 7K , 295K, 520K

Results

The main purpose of our project is to develop the G(r,E) analysis which can be transformed from the S(Q,E) map obtained by inelastic neutron scattering (INS) measurement. So far, the G(r,E) analysis is mainly applied to the disordered materials such as liquid and glass. Thus, it should be important to expand the applicability of G(r,E) analysis. In this study, we obtained INS spectra of both single crystalline (2014A $Ba_8Ga_{16}Sn_{30}$) and polycrystalline (2014B ScF_3) samples as preliminary data for G(r,E) analysis.

At first, the experimental results on single crystalline $Ba_8Ga_{16}Sn_{30}$ are given in Fig.1 which shows the neutron intensity map of transverse phonons along the [0LL] direction near (400) reciprocal lattice points. We have found that the data statistics and resolution in Fig.1 is too poor to obtain the correct G(r,E) data. Certainly, more intensity and sample amounts should be needed for G(r,E) analysis of single crystalline sample.

Next, we will discuss the data of polycrystalline ScF_3 which exhibits a large and isotropic negative thermal expansion (NTE). The INS measurement of this material performed by Li[1] has received a lot of attention[2]. Li and colleagues have shown the temperature dependent peak shifts for several phonons in density of states. However, our results were partially contradictory to their results. In particular, we found that the low-energy peak around 5 meV shows hardening behavior with increasing temperatures as shown in Fig.2, although Li and colleagues did not mention it.

１．研究成果概要（つづき） Outline of experimental results (continued).

These features are common in other NTE materials such as ZrW_2O_8 and Ag_2O. In order to complete our study, we have to be careful in several aspects. Firstly we will check the quality of ScF_3 powder sample by X-ray analysis.

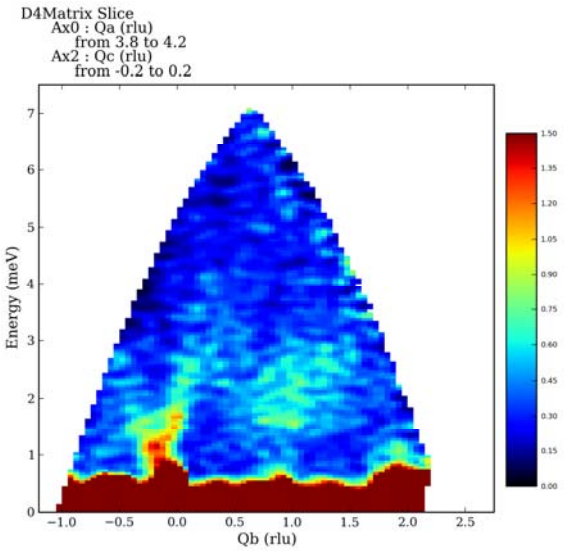

Fig.1: The neutron intensity map of single crystalline $Ba_8Ga_{16}Sn_{30}$. Transverse phonon along the [0LL] direction near (400) reciprocal lattice points is shown.

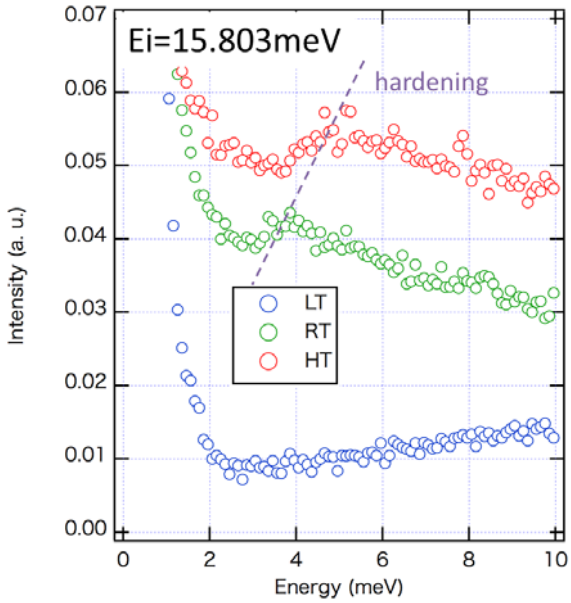

Fig.2: Temperature dependence of low-energy peak of ScF_3 powder. Here LT, RT and HT mean 7K, 295K and 520K, respectively.

[1] Chen W. Li *et al.*, Phys. Rev. Lett. **108** (2011) 195504.
[2] J. Paul Attfield, Nature **480** (2011) 465.

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